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Distributed Variational Inference in Sparse Gaussian Process Regression and Latent Variable Models

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Outline

Gaussian process regression and latent variable models

Why do we want to scale these?

Distributed inference

Utility in scaling-up GPs

New horizons in big data

GP regression & latent variable models

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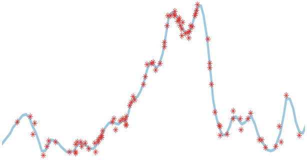
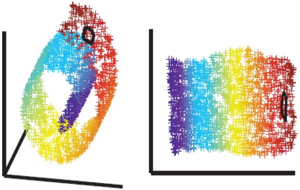
Gaussian processes (GPs) are a powerful tool for probabilistic inference over functions.

- GP regression captures non-linear functions
  - Can be seen as an infinite limit of *single layer neural networks*

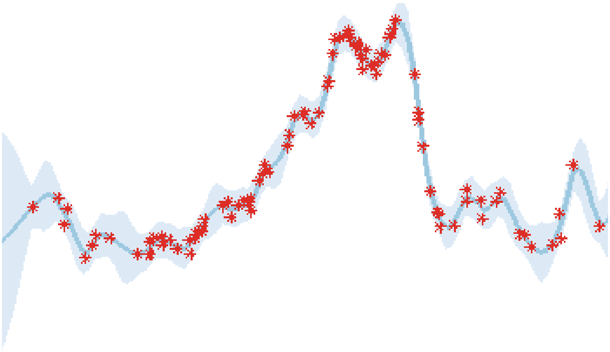


- GP latent variable models are an *unsupervised* version of regression, used for manifold learning
  - Can be seen as a non-linear generalisation of PCA



GPs offer:

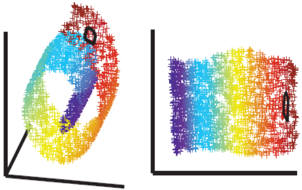
- uncertainty estimates,
- robustness to over-fitting,
- and principled ways for tuning hyper-parameters

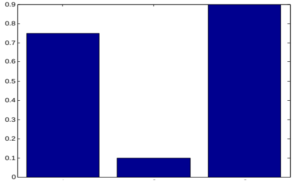


GP latent variable models

GP latent variable models are used for tasks such as...

- Dimensionality reduction
- Face reconstruction
- Human pose estimation and tracking
- Matching silhouettes
- Animation deformation and segmentation
- WiFi localisation
- State-of-the-art results for face recognition





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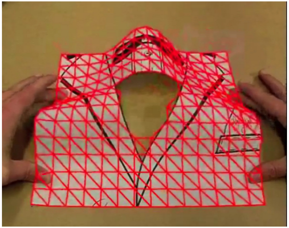

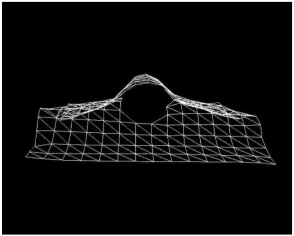

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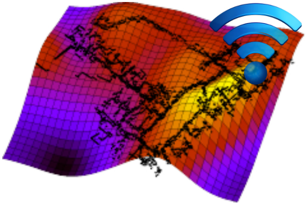

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Regression setting:

- Training dataset with N inputs $X \in \mathbb{R}^{N \times Q}$ (Q dimensional)
- Corresponding D dimensional outputs $F_n = \mathbf{f}(X_n)$
- We place a *Gaussian process prior* over the space of functions

$$\mathbf{f} \sim \mathcal{GP}(\text{mean } \mu(\mathbf{x}), \text{covariance } k(\mathbf{x}, \mathbf{x}'))$$

- This implies a joint Gaussian distribution over function values:

$$p(F|X) = \mathcal{N}(F; \mu(X), K), \quad K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

- Y consists of noisy observations, making the functions F latent:

$$p(Y|F) = \mathcal{N}(Y; F, \beta^{-1} I_n)$$

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GP latent variable models

Latent variable models setting:

- Infer both the inputs, which are now latent, and the latent function mappings at the same time
- Model identical to regression, with a prior over now latents X

$$X_n \sim \mathcal{N}(X_n; 0, I), \quad F(X_n) \sim \mathcal{GP}(0, k(X, X)), \quad Y_n \sim \mathcal{N}(F_n, \beta^{-1} I)$$

- In approximate inference we look for variational lower bound to:

$$p(Y) = \int p(Y|F)p(F|X)p(X)\mathrm{d}(F, X)$$

- This leads to Gaussian approximation to the posterior over X

$$q(X) :\approx p(X|Y)$$

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Why do we want to scale GPs?

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- Naive models are often used with big data (linear regression, ridge regression, random forests, etc.)
- These don't offer many of the desirable properties of GPs (non-linearity, robustness, uncertainty, etc.)
- Scaling GP regression and latent variable models allows for *non-linear regression, density estimation, data imputation, dimensionality reduction, etc.* on big datasets

Problem – time and space complexity

- Evaluating $p(Y|X)$ directly is an expensive operation
- Involves the inversion of the n by n matrix K
- requiring $\mathcal{O}(n^3)$ time complexity

Sparse approximation!

Solution – sparse approximation!

- A collection of M "inducing inputs" – a set of points in the same input space with corresponding values in the output space.
- These summarise the characteristics of the function using less points than the training data.
- Given the dataset, we want to learn an optimal subset of inducing inputs.
- Requires $\mathcal{O}(nm^2 + m^3)$ time complexity.

[Quiñonero-Candela and Rasmussen, 2005]

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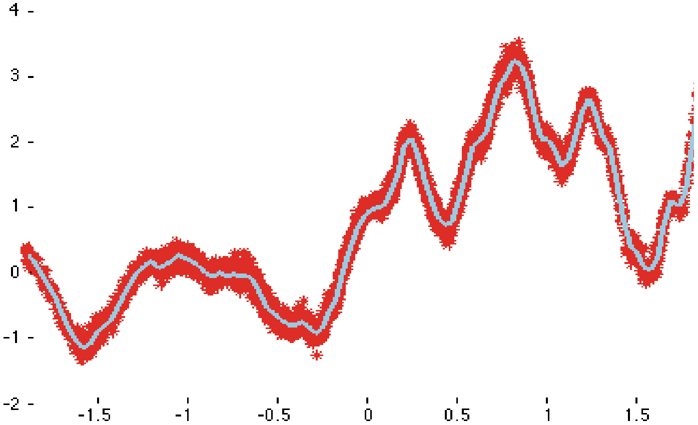
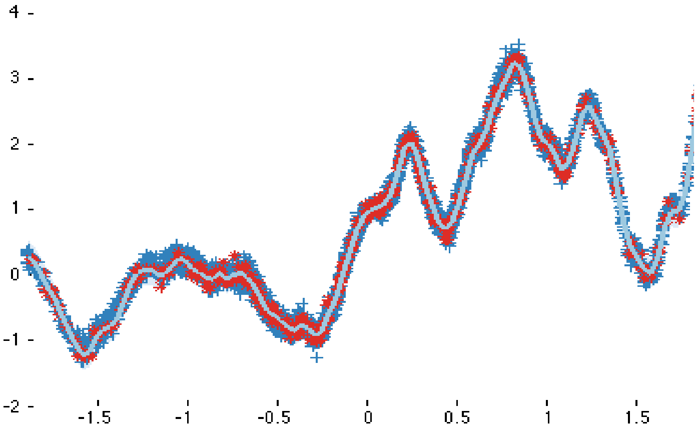
Sparse approximation in pictures:



Regression on 5000 points dataset

Sparse approximation in pictures:

- We can summarise the data using a small number of points



Regression on 500 points subset (in red)

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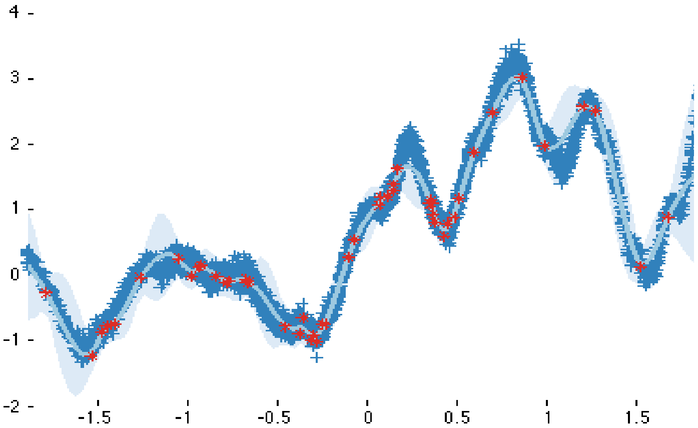

Regression on 50 points subset (in red)

Distributed Inference in GPs

Why do we want distributed inference?

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Usual datasets used with full GPs [$\mathcal{O}(n^3)$]

Why do we want distributed inference?

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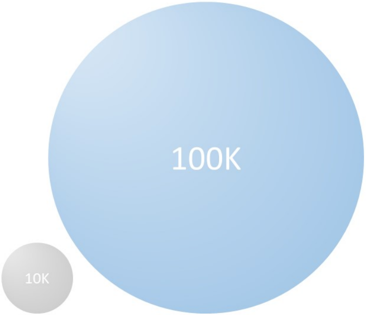
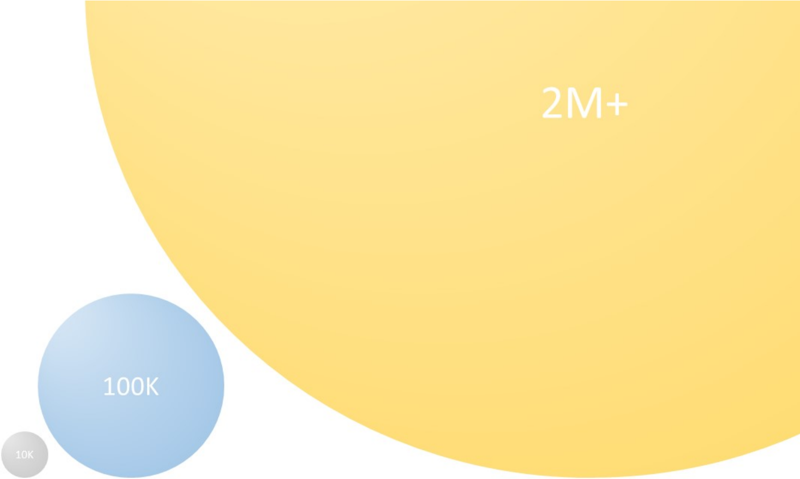
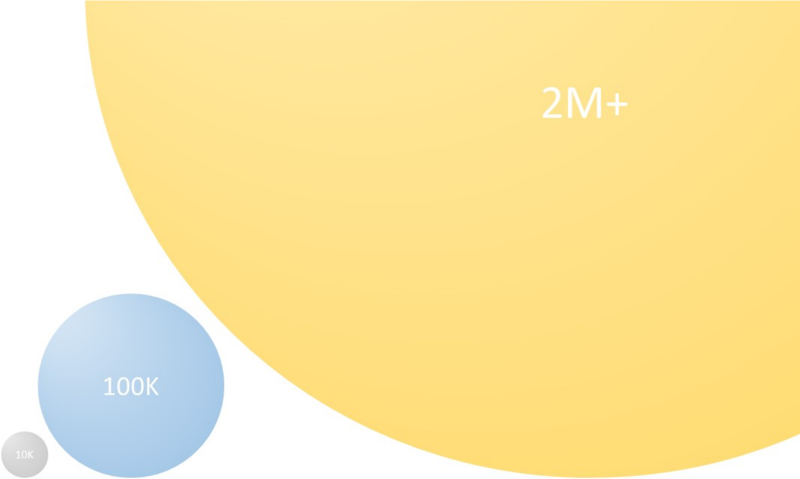


Usual datasets used with Sparse GPs [$\mathcal{O}(nm^2 + m^3)$, $m << n$]

Why do we want distributed inference?



Big data



Distributed Sparse GPs – $\mathcal{O}(\frac{nm^2}{T} + m^3) = \mathcal{O}(n + m^3)$,
for $T = m^2$ nodes, $m << n$

Distributing the inference

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- The data points become independent of one another given the inducing inputs
- We can write the evidence lower bound as:

$$\log p(Y) \geq \sum_{i=1}^{n} \int q(\mathbf{u})q(X_i)p(F_i|X_i,\mathbf{u}) \log p(Y_i|F_i) \mathrm{d}(F_i, X_i, \mathbf{u}) - KL(q(\mathbf{u})||p(\mathbf{u})) - KL(q(X)||p(X))$$

  with inducing inputs $\mathbf{u}$ and approximating distributions $q(\cdot)$
- We can analytically integrate out $q(\mathbf{u})$ and still keep a factorised form
- We can compute each term in the factorised form independently of the others with the *Map-Reduce framework*.

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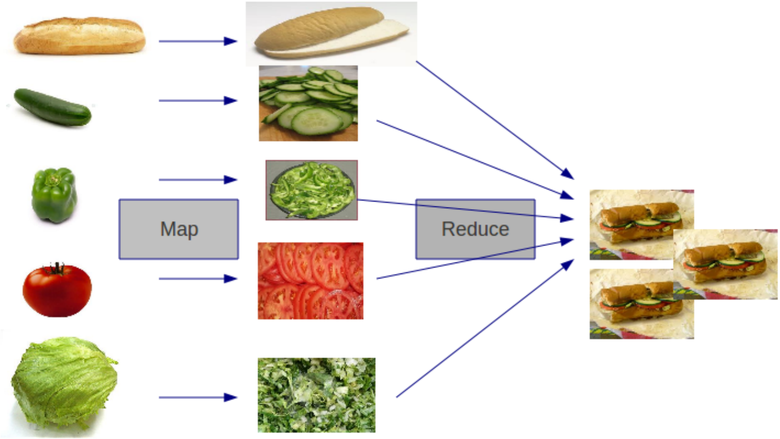
Map-Reduce framework



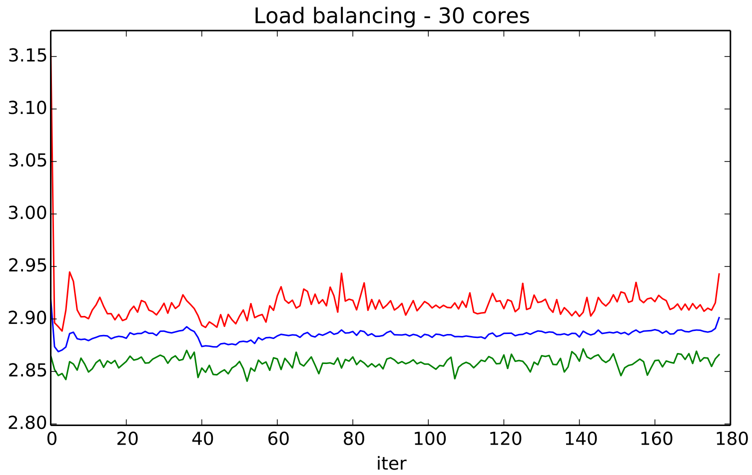
[http://mohamednabeel.blogspot.co.uk/]

Characteristics of distributed inference

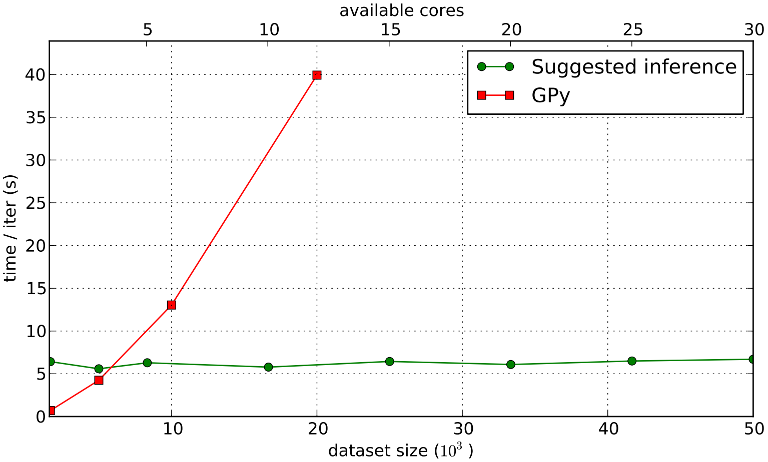
The inference procedure should:

- distribute the computational load evenly across nodes,
- scale favourably with the number of nodes,
- and have low overhead in the global steps.

Characteristics of distributed inference



Distribution of computational load



Scalability with the number of nodes

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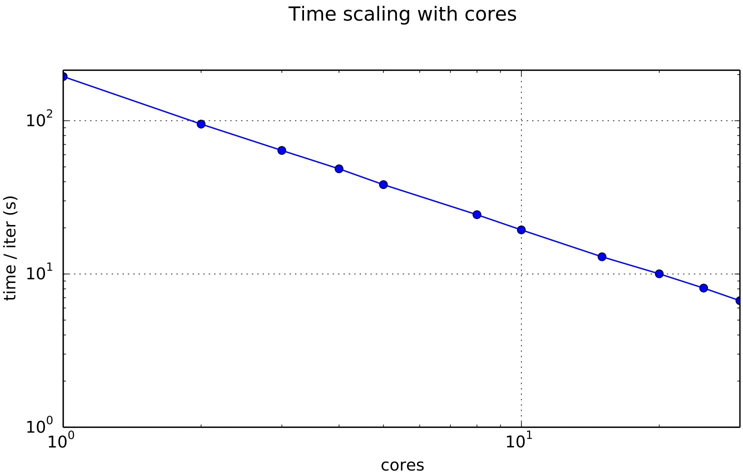

Negligible overhead in the global steps (constant time – $\mathcal{O}(m^3)$)

Utility in scaling-up GPs

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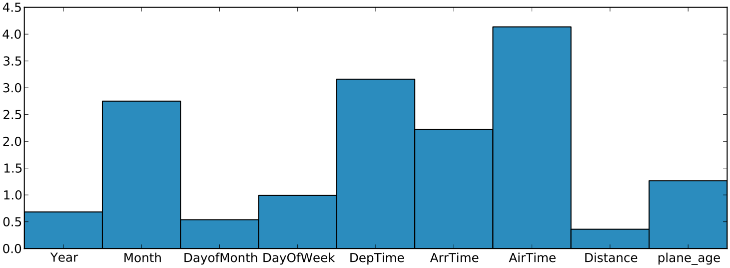
- We want to predict flight delays from various flight-record characteristics (flight date and time, flight distance, etc.)
- Can we improve on GP prediction using increasing amounts of data?
- We use different subset sizes of data: 7K, 70K, and 700K

Utility in scaling-up GPs

Size	7K	70K	700K
Dist GP	**33.56**	**33.11**	**32.95**

Root mean square error (RMSE) on flight dataset 7K-700K

- With more data we can learn better inducing inputs!



ARD parameters for flight 700K

Utility in scaling-up GPs

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GP latent variable model on the full MNIST dataset (60K, 784 dim.):

- Used a density model for each digit
- No pre-processing (the model is non-specialised)
- Trained the models on 10K and all 60K points

Size	10K	60K
Dist GP	**8.98%**	**5.95%**

Classification error on a subset and full MNIST

- Improvement of 3.03 percentage points
- Training on the full MNIST dataset took 20 minutes for the longest running model

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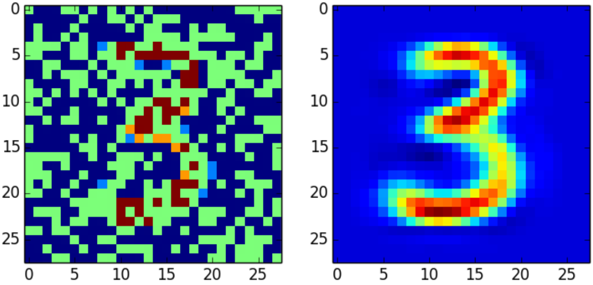
But these models give us much more...

- The MNIST trained models are density estimation models
- They allow us to perform image imputation,
- Generate new digits by sampling from the posterior, etc.



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Furthermore, real big data is complex and non-linear – and naive models may under-perform on it

- Back to flight regression –
- Flight 2M dataset compared to common approaches in big data:

Dataset	Mean	Linear	Ridge	RF	Dist GP
Flight 2M	38.92	37.65	37.65	37.33	**35.31**

RMSE of regression over flight data with 2M points

- These are just error rates – we can do much more with GPs
  - robust, offer uncertainty bounds, etc.

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Conclusions

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- We showed that the inference scales well with data and computational resources
- We demonstrated the utility in scaling GPs to big data
- The results show that GPs perform better than many common models often used for big data

Conclusions

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- Developing the inference we wrote an introductory tutorial [Gal and van der Wilk, 2014] with detailed derivations
- The code developed is open source[1]
  - 300 lines of Python with detailed and documented examples
- Pointers between equations in the tutorial and in code

B.2.2 Partial derivatives with respect to σ_f^2

The partial derivative $\frac{\partial K_{mm}}{\partial \sigma_f^2}$

$$\left(\frac{\partial K_{mm}}{\partial \sigma_f^2}\right)_{mm'} = \frac{k(Z_m, Z_{m'})}{\sigma_f^2} \quad \text{(B.54)}$$

The partial derivative $\frac{\partial \left\langle K_{ii}^{X_i} \right\rangle_{q(X_i)}}{\partial \sigma_f^2}$

$$\frac{\partial \left\langle K_{ii}^{X_i} \right\rangle_{q(X_i)}}{\partial \sigma_f^2} = 1 \quad \text{(B.55)}$$

```
########################################
# grad_sf2 and necessary functions
########################################

def dKmm_dsf2(self):
    # Eqn (B.54)
    return self.Kmm / self.hyp.sf**2

def dexp_K_ii_dsf2(self):
    # Eqn (B.55)
    return self.local_N
```

[1] See https://github.com/markvdw/GParML